Resonant Dissociative Recombination: H_3^+ and HeH^{+*}

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Formal resonance theory provides an elegant and potentially exact framework for describing the process of resonant dissociative recombination. In most treatments, semi-empirical methods have been used to derive the required resonance parameters. We show that *ab initio* theory can provide a quantitative treatment of resonant dissociative recombination. The resonance positions and widths as a function of internuclear separation are obtained via accurate electron scattering calculations using the complex Kohn method. This information was used as input to a wave packet calculation for the dissociation dynamics. The method is illustrated by two examples. First, H_3^+, a triatomic system where two nuclear degrees of freedom must be included to correctly describe the dissociation dynamics, and HeH^+, where a proper multi-channel treatment of the high-lying resonances is needed to achieve quantitative agreement with experiment.